

Supplementary Table S2

(Foods)

Insights on single-dose espresso coffee capsules' volatile profile: from ground powder volatiles to prediction of espresso brew aroma properties

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Table S2. GC × GC peak areas of 390 volatile compounds putatively identified in 8 roasted ground capsule-coffee powders and respective espresso brews, using HS-SPME/GC × GC-ToFMS.

Peak no.	Compound	Powder						Brew									
		Dec	1	2	3	4	5	6	Sup	Dec	1	2	3	4	5	6	Sup
	Acids	1.56×10 ⁹ (17.9)	1.37×10 ⁹ (23.2)	1.57×10 ⁹ (15.5)	1.92×10 ⁹ (8.6)	1.66×10 ⁹ (34.8)	1.56×10 ⁹ (5.0)	1.62×10 ⁹ (25.2)	1.30×10 ⁹ (54.8)	2.88×10 ⁸ (20.3)	2.55×10 ⁸ (27.3)	1.55×10 ⁸ (38.1)	5.30×10 ⁷ (30.8)	2.71×10 ⁸ (19.0)	2.87×10 ⁸ (2.0)	2.01×10 ⁸ (17.6)	1.07×10 ⁸ (63.1)
<i>Aliphatics</i>																	
1	Acetic acid	1.35×10 ⁹	9.47×10 ⁸	1.07×10 ⁹	1.43×10 ⁹	1.10×10 ⁹	1.08×10 ⁹	1.18×10 ⁹	8.69×10 ⁸	2.82×10 ⁸	2.38×10 ⁸	1.37×10 ⁸	4.90×10 ⁷	2.55×10 ⁸	2.71×10 ⁸	1.93×10 ⁸	9.90×10 ⁷
2	Propanoic acid	7.14×10 ⁷	6.02×10 ⁷	9.17×10 ⁷	4.15×10 ⁷	1.25×10 ⁸	2.68×10 ⁷	2.90×10 ⁷	5.04×10 ⁷	4.73×10 ⁵	1.32×10 ⁵	1.32×10 ⁵	9.86×10 ⁵	2.05×10 ⁶	2.23×10 ⁶	1.32×10 ⁵	
3	Butanoic acid	4.27×10 ⁶	4.50×10 ⁶	7.42×10 ⁶	5.96×10 ⁶	1.31×10 ⁷	7.72×10 ⁶	6.96×10 ⁶	5.90×10 ⁶	4.59×10 ⁴	4.59×10 ⁴	1.07×10 ⁵	4.59×10 ⁴	4.59×10 ⁴	4.59×10 ⁴	4.59×10 ⁴	
4	Isovaleric acid	1.25×10 ⁸	3.60×10 ⁸	4.11×10 ⁸	4.40×10 ⁸	4.19×10 ⁸	4.43×10 ⁸	3.98×10 ⁸	3.76×10 ⁸	5.34×10 ⁶	1.71×10 ⁷	1.80×10 ⁷	3.81×10 ⁶	1.56×10 ⁷	1.38×10 ⁷	6.02×10 ⁶	7.71×10 ⁶
	Alcohols	5.50×10 ⁷ (4.0)	1.06×10 ⁸ (7.7)	1.14×10 ⁸ (8.5)	1.16×10 ⁸ (18.9)	7.20×10 ⁷ (24.7)	1.11×10 ⁸ (7.9)	8.49×10 ⁷ (8.1)	7.32×10 ⁷ (19.7)	5.94×10 ⁷ (5.1)	1.30×10 ⁸ (11.3)	7.40×10 ⁷ (29.2)	3.90×10 ⁷ (3.3)	1.14×10 ⁸ (7.0)	9.14×10 ⁷ (14.7)	4.58×10 ⁷ (12.5)	
<i>Aliphatics</i>																	
5	2-Methyl-1-propanol	4.95×10 ⁵	6.61×10 ⁵	1.60×10 ⁶	4.55×10 ⁵	1.80×10 ⁵	1.44×10 ⁶	7.85×10 ⁵	4.81×10 ⁵	3.83×10 ⁵	4.95×10 ⁵	3.69×10 ⁵	3.44×10 ⁵	5.35×10 ⁵	3.77×10 ⁵	3.23×10 ⁵	1.50×10 ⁵
6	3-Buten-1-ol	1.60×10 ⁶	1.30×10 ⁶	1.65×10 ⁶	8.81×10 ⁵	1.60×10 ⁵	1.48×10 ⁶	1.25×10 ⁶	1.17×10 ⁶	n.d.							
7	3-Methyl-3-buten-1-ol	8.77×10 ⁶	1.27×10 ⁷	1.64×10 ⁷	1.26×10 ⁷	6.67×10 ⁶	2.48×10 ⁷	1.72×10 ⁷	6.80×10 ⁶	9.49×10 ⁶	8.06×10 ⁶	5.09×10 ⁶	1.85×10 ⁶	8.01×10 ⁶	1.05×10 ⁷	6.78×10 ⁶	1.75×10 ⁶
8	2-Methyl-1-butanol	2.10×10 ⁶	1.49×10 ⁷	2.46×10 ⁷	1.71×10 ⁷	2.34×10 ⁶	1.95×10 ⁷	8.09×10 ⁶	3.28×10 ⁶	4.24×10 ⁶	7.99×10 ⁶	6.15×10 ⁶	3.47×10 ⁶	1.00×10 ⁷	1.09×10 ⁷	6.64×10 ⁶	2.85×10 ⁶
9	1-Pentanol	3.33×10 ⁶	2.40×10 ⁶	2.91×10 ⁶	2.17×10 ⁶	2.99×10 ⁶	5.22×10 ⁶	4.63×10 ⁶	2.01×10 ⁶	1.40×10 ⁶	2.43×10 ⁶	1.36×10 ⁶	6.25×10 ⁵	5.11×10 ⁶	5.17×10 ⁶	2.90×10 ⁶	6.72×10 ⁵
10	3-Methyl-2-buten-1-ol	3.29×10 ⁶	6.58×10 ⁶	7.74×10 ⁶	6.01×10 ⁶	3.75×10 ⁶	7.85×10 ⁶	1.00×10 ⁷	3.55×10 ⁶	3.08×10 ⁶	4.13×10 ⁶	2.32×10 ⁶	1.20×10 ⁶	3.76×10 ⁶	4.63×10 ⁶	4.07×10 ⁶	9.92×10 ⁵
11	2-Hexanol	2.69×10 ⁵	6.51×10 ⁵	5.68×10 ⁵	6.45×10 ⁵	2.32×10 ⁵	3.57×10 ⁵	1.55×10 ⁵	3.46×10 ⁵	4.60×10 ⁵	1.31×10 ⁶	5.51×10 ⁵	3.02×10 ⁵	8.88×10 ⁵	5.26×10 ⁵	1.90×10 ⁵	2.93×10 ⁵
12	2-Heptanol	1.33×10 ⁷	3.03×10 ⁷	2.54×10 ⁷	2.84×10 ⁷	1.44×10 ⁷	1.66×10 ⁷	8.67×10 ⁶	2.18×10 ⁷	2.12×10 ⁷	6.91×10 ⁷	3.42×10 ⁷	2.06×10 ⁷	5.00×10 ⁷	3.22×10 ⁷	1.04×10 ⁷	2.16×10 ⁷
13	1-Octen-3-ol	1.12×10 ⁷	1.61×10 ⁷	8.38×10 ⁶	1.47×10 ⁷	1.27×10 ⁷	1.10×10 ⁷	1.49×10 ⁷	5.65×10 ⁶	1.27×10 ⁷	2.35×10 ⁷	1.58×10 ⁷	7.29×10 ⁶	2.66×10 ⁷	1.72×10 ⁷	1.11×10 ⁷	7.92×10 ⁶
14	2-Ethyl-1-hexanol	1.46×10 ⁶	1.65×10 ⁶	1.92×10 ⁶	1.90×10 ⁶	4.04×10 ⁶	1.44×10 ⁶	1.43×10 ⁶	1.69×10 ⁶	1.66×10 ⁶	1.35×10 ⁶	1.65×10 ⁶	1.17×10 ⁶	8.88×10 ⁵	8.71×10 ⁵	5.62×10 ⁵	5.68×10 ⁵
15	1-Octanol	6.00×10 ⁵	8.53×10 ⁵	6.04×10 ⁵	1.15×10 ⁶	1.10×10 ⁶	1.07×10 ⁶	7.09×10 ⁵	1.12×10 ⁶	1.23×10 ⁶	2.32×10 ⁶	1.38×10 ⁶	8.71×10 ⁵	1.67×10 ⁶	2.32×10 ⁶	1.19×10 ⁶	5.97×10 ⁵
<i>Aromatics</i>																	
16	2-Phenylethanol	8.60×10 ⁶	1.74×10 ⁷	2.23×10 ⁷	3.05×10 ⁷	2.34×10 ⁷	2.03×10 ⁷	1.71×10 ⁷	2.53×10 ⁷	3.57×10 ⁶	9.46×10 ⁶	5.10×10 ⁶	1.31×10 ⁶	6.42×10 ⁶	6.75×10 ⁶	1.63×10 ⁶	2.12×10 ⁶
	Aldehydes	4.31×10 ⁸ (7.7)	3.33×10 ⁸ (9.0)	3.40×10 ⁸ (16.1)	3.52×10 ⁸ (19.7)	2.78×10 ⁸ (26.3)	4.68×10 ⁸ (39.6)	3.65×10 ⁸ (9.1)	3.13×10 ⁸ (27.2)	1.08×10 ⁹ (3.1)	9.46×10 ⁸ (15.6)	6.25×10 ⁸ (22.1)	4.10×10 ⁸ (2.3)	8.59×10 ⁸ (8.4)	7.81×10 ⁸ (6.2)	5.36×10 ⁸ (16.9)	3.68×10 ⁸ (5.2)
<i>Aliphatics</i>																	
17	Acetaldehyde	1.81×10 ⁷	1.49×10 ⁷	1.46×10 ⁷	2.50×10 ⁷	1.54×10 ⁷	1.99×10 ⁷	1.18×10 ⁷	1.05×10 ⁷	1.30×10 ⁷	1.14×10 ⁷	3.01×10 ⁶	6.85×10 ⁶	1.23×10 ⁷	1.23×10 ⁷	8.83×10 ⁶	5.40×10 ⁶

